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IMPROVED TWO-DIMENSIONAL-KINETICS

COMPUTER PROGRAM

NAS8-35931

Third Quarterly Progress Report

1 July 1984 through 30 September 1984

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IMPROVED TWO-DIMENSIONAL-KINETICS COMPUTER PROGRAM

1.0 BACKGROUND

Future Orbit Transfer Vehicles (OTV) presently under consideration need rocket engines delivering a high specific impulse. This high performance can be obtained with large area ratio thrust chambers using oxygen with either hydrogen or hydrocarbon fuels. In the projected nozzles the combustion products are expanded to low pressure and temperature levels at high Mach-number flow, a domain which has not been experienced with existing rocket engines.

Some modifications have recently been incorporated in the Two-Dimensional-Kinetics (TDK) computer program, such as: Condensed phase flow simulation, treatment of shock waves induced by the wall curvature, and the coupling of the TDK code with the Boundary Layer Module (BLM) for an improved thrust chamber specific impulse prediction.

Recent boundary layer calculations for large area ratio nozzles have revealed that the boundary layer becomes very thick in the region of high Mach-numbers. This result is quite different from rocket engines built up to now and requires an examination of the existing thrust loss calculation method due to the viscous effects adjacent to the wall. Furthermore, the knowledge of the Knudsen-number is desirable which differentiates between continuum, slip and free molecular flow, and thereby identified when the analysis, presently based on Newtonian fluid flow, becomes questionable or invalid.

In order to obtain highly accurate performance predictions, the best supporting data for equilibrium and finite rate chemistry must be prepared. Furthermore, the large area ratio nozzles require many more calculation steps to cover the complete nozzle flow field. This increases computation time significantly and favors an error accumulation which should be reduced as much as possible. Another point of importance connected with the OTV is the existence of ionized combustion products which permits vehicle tracing or interferes with the transfer of communication or command signals.

The current effort of shock wave modeling induced by the curvature of the wall should be expanded to permit the shock simulation caused by wall contour discontinuities. Also the Mach shock existence in the center of the flow field interacting with other shocks as well as the analytical treatment of multiple shock waves may significantly affect the interior nozzle flow and associated performance and need to be simulated.

2.0 OBJECTIVE

The objective of this effort is to increase the analytical capability of the existing TDK/BLM computer program for performance of OTV thrust chambers. Areas which need further examination and improvement are the thick boundary layer inviscid core flow interaction and the related thrust loss calculation. To warrant highly accurate results the provision of the best available program input data is mandatory as well as the use of sophisticated modeling techniques to reduce computation time with advanced error control criteria. The simulation of wall shocks, Mach-shocks in addition to shocks induced by large concave wall curvature is essential since this interaction with each other produces flow field changes which in turn affect the nozzle performance.

3.0 WORK PERFORMED DURING THE REPORTING PERIOD

The program plan for this work is presented in Figure A. Progress in each of the work tasks during the reporting period is presented in the sub-paragraphs 3.1 through 3.5.

3.1 TDK-BLM INTERFACE

Interaction between the inviscid core flow and the wall boundary layer is expressed through 1st order by the definition of displacement thickness, δ^*. We have rederived δ^* and θ for the nozzle wall boundary layer situation for the purpose of obtaining a more accurate representation, especially when the boundary layer is thick. In particular the radial coordinate, r, has not been factored. Integral expressions are obtained that are somewhat different than the classical expressions. For example, the expression for δ^* is found to be:

$$\delta_a^* = \int_0^\delta \left(1 - \frac{\rho u r}{\rho_e u_e \bar{r}_{1e}}\right) dy , \quad \bar{r}_{1e} = \frac{r_1 + r_e}{2} .$$

This is an implicit expression, since conditions at e are displaced from the wall by a distance δ_a^*. The subscript 1 refers to a displacement equal to the velocity thickness. It is found that the boundary layer thrust deficit does not use this integral, but a somewhat different integral, as follows:

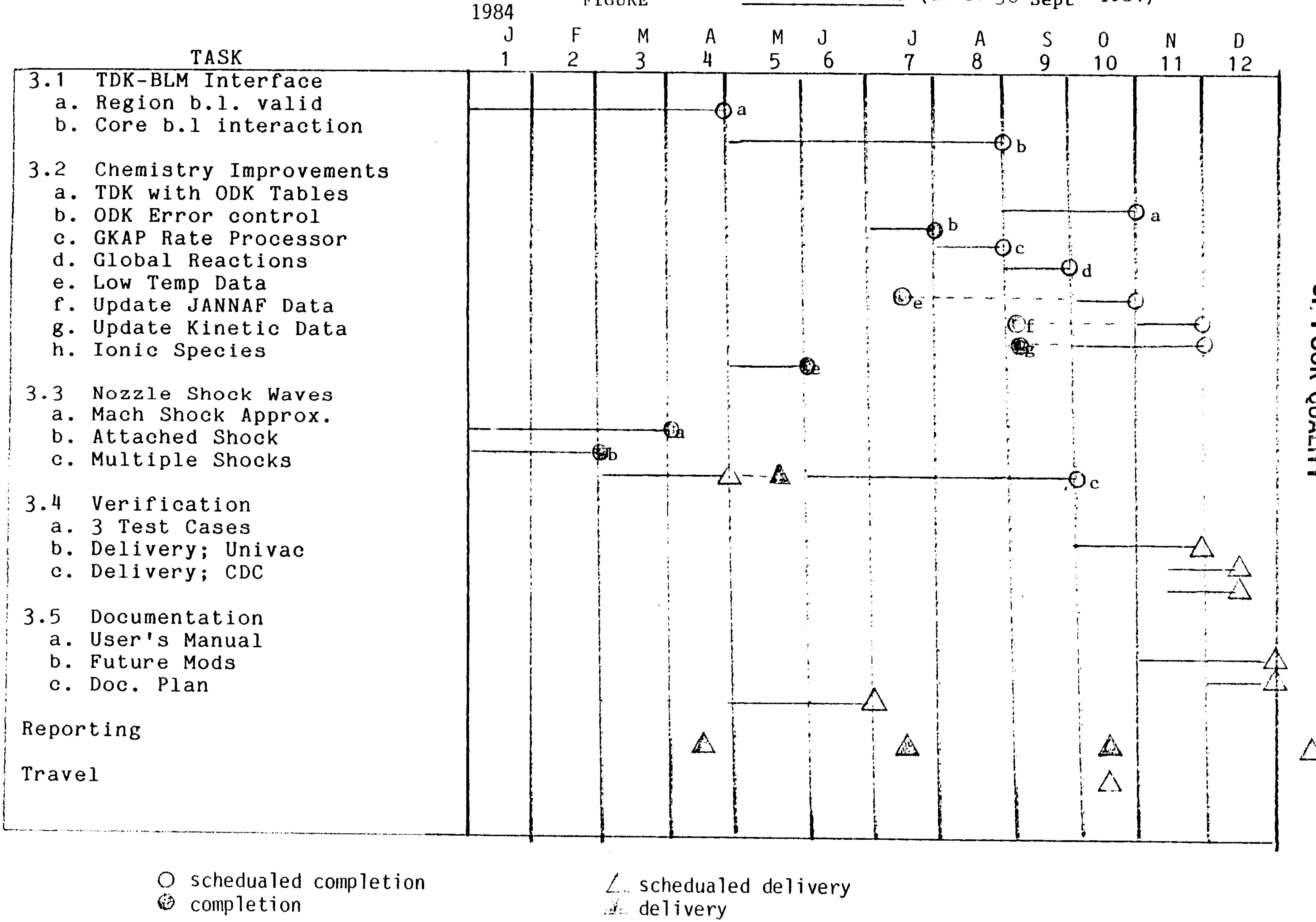
$$\delta_b^* = \int_0^\delta \left(1 - \frac{\rho u r}{\rho_e u_e \bar{r}_{1w}}\right) dy , \quad \bar{r}_{1w} = \frac{r_1 + r_w}{2} .$$

This is a explicit expression. The subscript w refers to conditions at the wall.

Similar remarks apply to the momentum thickness, Θ.

FIGURE

PROGRAM PLAN (as of 30 Sept 1984)



3.2 CHEMISTRY IMPROVEMENTS

Task 3.2b, ODK Error Control

This task was completed during the reporting period. The numerical integration method was rederived, and is attached as Appendix A.

A new error control formula was derived that is based on an estimate of the absolute error for the integration step. This is done by evaluating the next term (3rd order) in the series expansion. The absolute error is converted to a relative error, unless the variable is too small, in which case the absolute error is used. The error term is used to control step size doubling or halving as shown in the attached write-up for subroutine INT.

It was found that accurate integration of the differential equations requires consistancy in the nozzle cross-sectional area and its derivatives. Values of $A(x)$, dA/dx and d^2A/dx^2 are required for the supersonic flow region. The subroutine used for interpolation, SPLN, was modified so that y, y', and y'' are found by cubic, parabolic and linear interpolation, respectively, such that y' is the integral y'', etc.

The method was tested using the TDK analysis for the SSME. Plots describing the supersonic wall contour and its derivatives are shown in Figure 1. Local error vs. x/y* and step size vs. x/y* are plotted in Figure 2 and 3. The maximum step size was input as .2. The run time for this case was 25 seconds on the VAX 780. Previous to implementing the new error control method, this case required 127 CPU seconds. The old error control forced a fixed step size of .005. Thus, the new method gives a factor of 5 improvements on run time for this case.

The success of this task will prove very useful when task 3.2a; TDK with ODK Tables, is done since the ODK computer time has been reduced substantially.

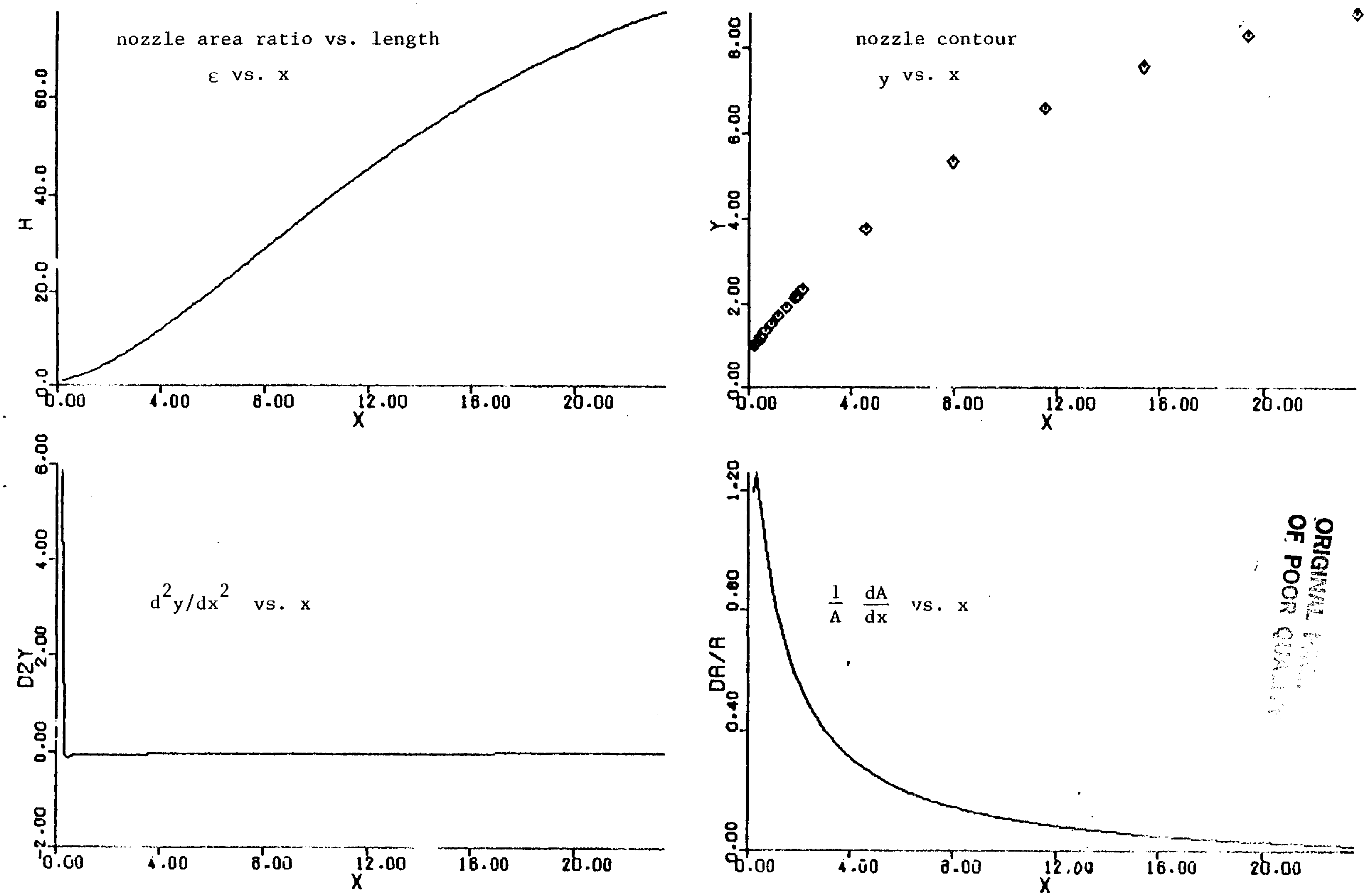


Figure 1: Plots Describing the Supersonic Nozzle Wall Contour
(x and y are divided by the throat radius)

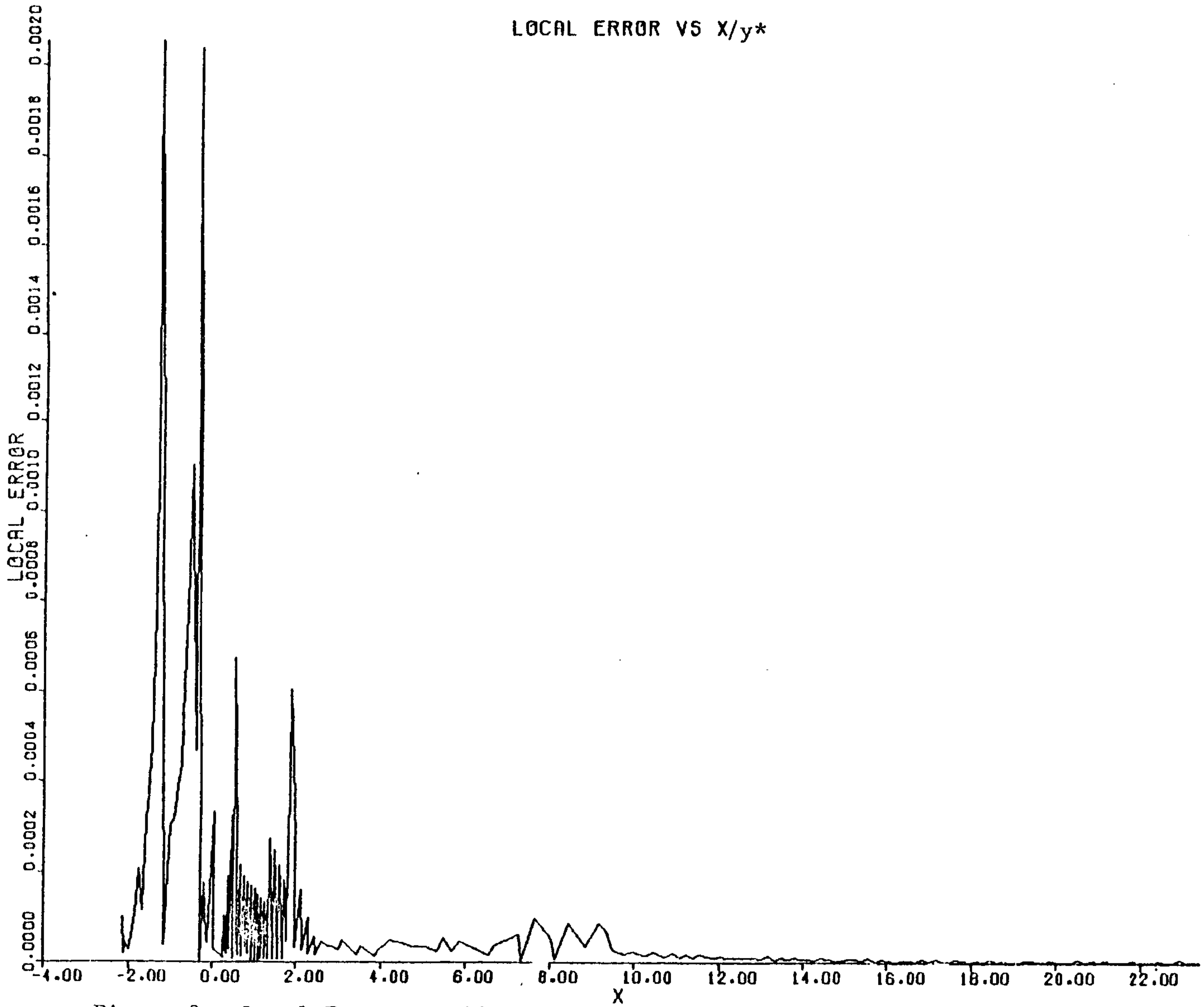


Figure 2: Local Error vs. Distance

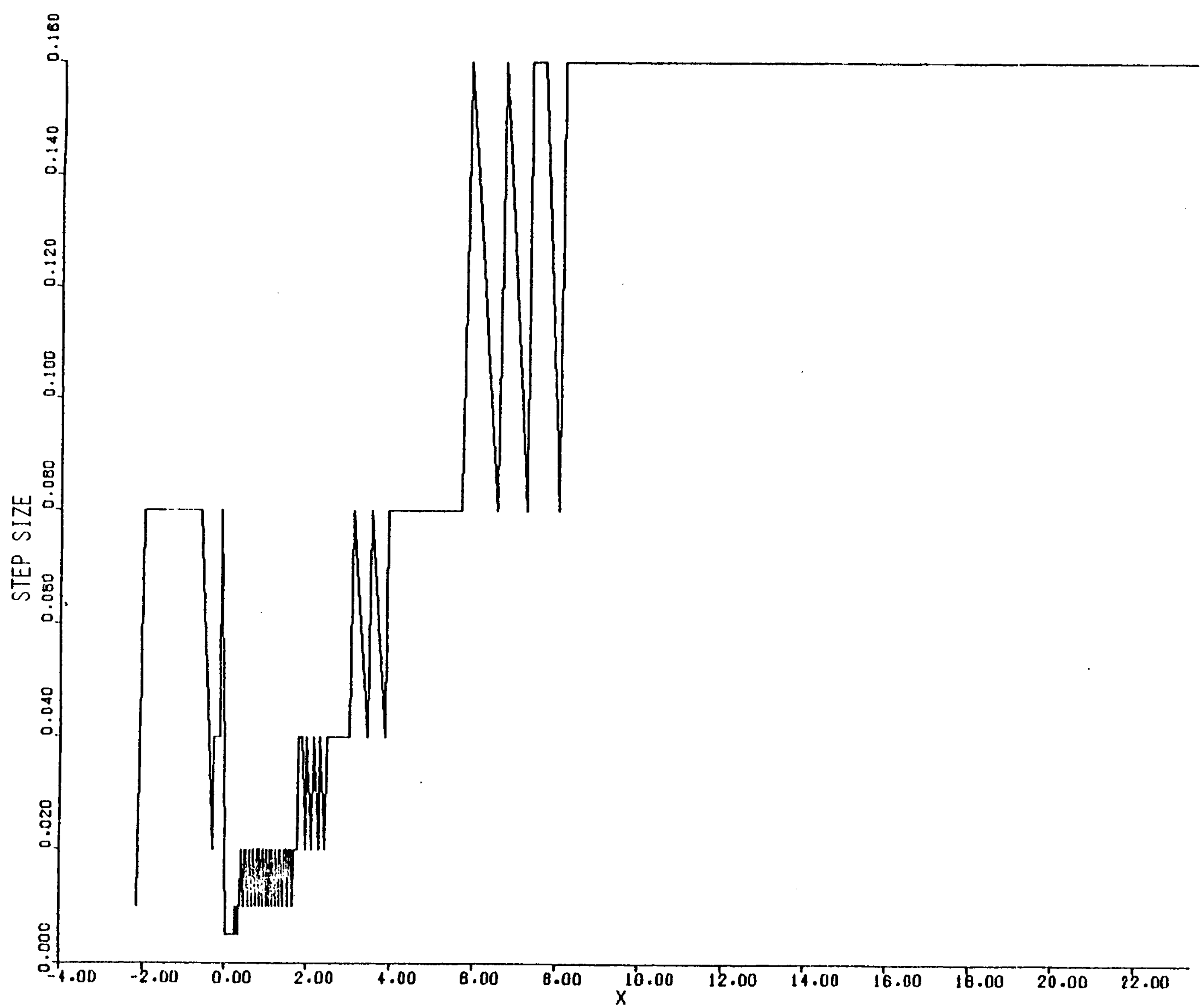


Figure 3: Step Size vs. Distance

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SUBROUTINE INT

Provides control for the implicit integration procedure, determines the proper set of nonhomogeneous equations to solve, and, after each integration step, computes the next integration step size according to the following relations:

$$h_{n+2} = 2h_{n+1}, \qquad \left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3y_{max}}\right|_{MAX} < \frac{\delta}{20}$$

$$h_{n+2} = \frac{1}{2}h_{n+1}, \qquad \left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3y_{max}}\right|_{MAX} > \delta$$

$$h_{n+2} = h_{n+1}, \qquad \frac{\delta}{20} \le \left|\frac{k_{i,n+1} - 2k_{i,n} + k_{i,n-1}}{3y_{max}}\right|_{MAX} \le \delta$$

where

$$y_{max} = \max \left[|y_{i,n}|, 10^{-5} \right] \qquad ; i = 1,2,\ldots \text{NSP}+3$$

On option, (JF=1) only the fluid dynamic variables are used in determining the next integration step size.

If the step size is halved for the fourth step, the integration is restarted using one-half the original step size.

The correspondence between equation number and physical property is:

Equation Number	Property
1	Velocity of Gas
2	Density of Gas
3	Temperature of Gas
4 NSP+3	Gaseous species mass fraction (1...NSP) correspondence to (4...NSP + 3)

When the flow is supersonic, continuity is used to control the integration step size to insure that:

$$\left|\frac{(\rho VA)_{N+1} - (\rho VA)_N}{(\rho VA)_{N+1}}\right| < \text{CØNDEL}$$

where CØNDEL is an input relative criterion with a default value 10^{-5}.

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Task 3.2e, Low Temperature Data

This task has been completed except for adding a default low temperature data file to the program. Section 6.1.1 of the TDK manual has been rewritten to describe the usage of this data, and is attached as Appendix B. Note that only Cp vs T is to be input.

Example, plots obtained from the method are shown in Figures 4,5, and 6. The properties are for the species H_2. Figure 4 shows the input table of Cp vs. T. Figures 5 and 6 show the integrated values derived from Figure 4 for S and h vs. T.

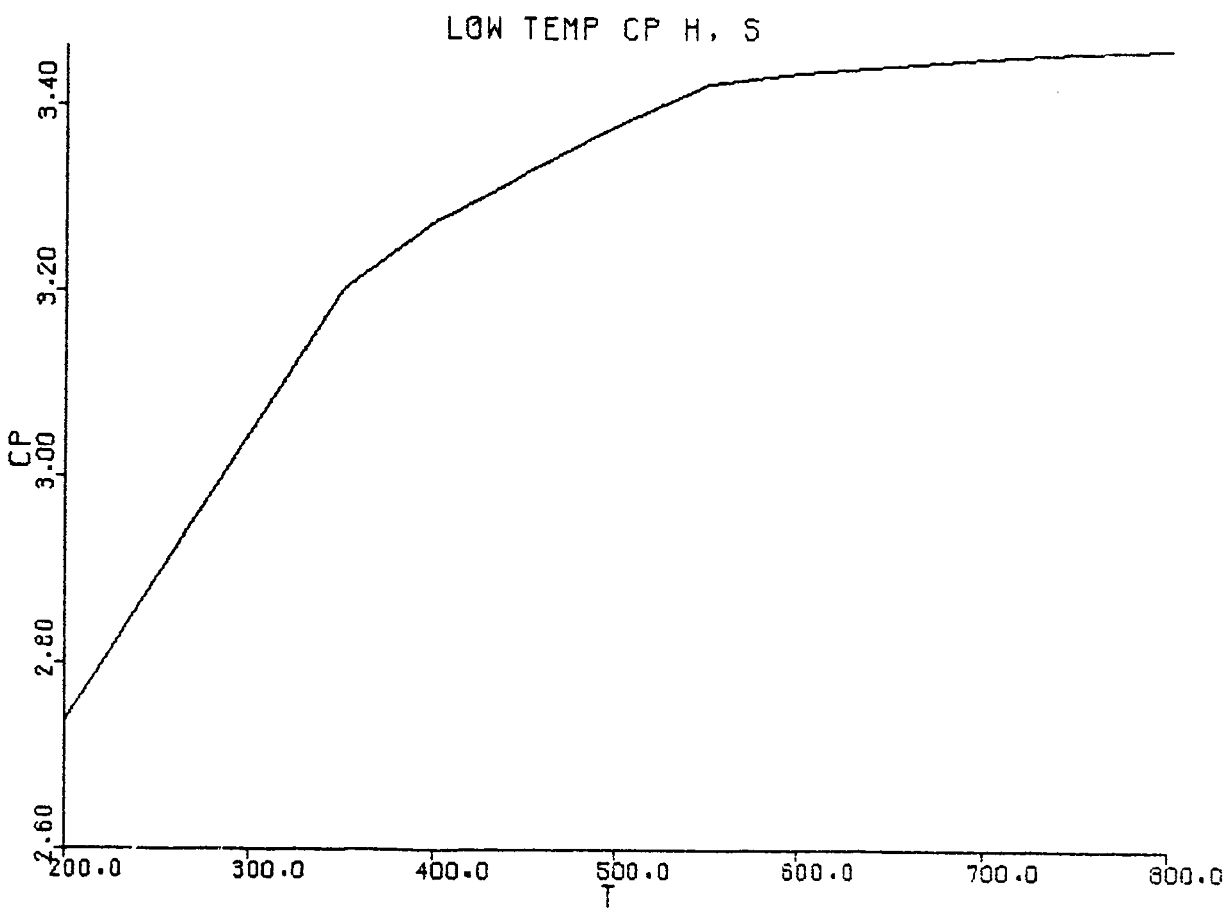

Figure 4: C_p vs T for H_2

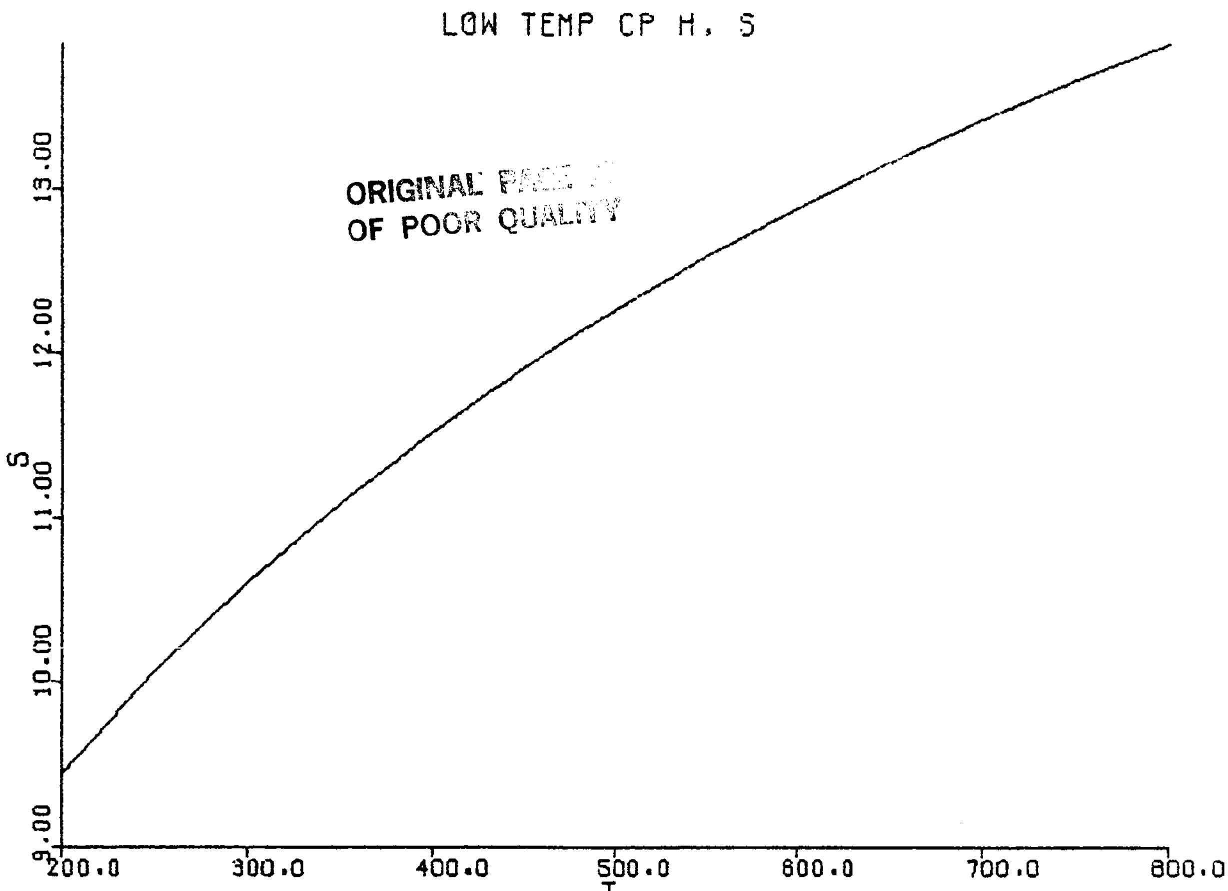

Figure 5: S vs T for H_2

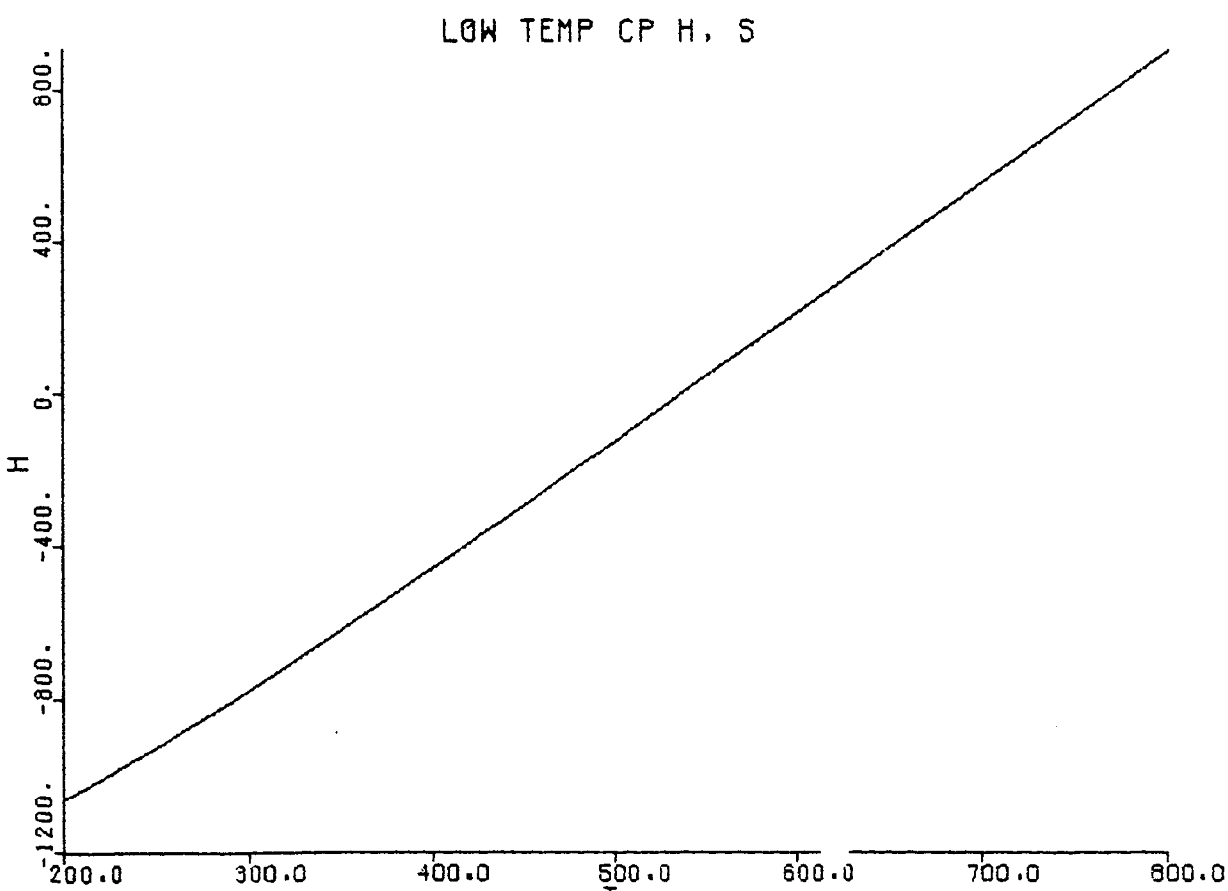

Figure 6: H vs T for H_2

Task 3.2f, Update JANNAF Data

The JANNAF thermochemical Data has been updated by obtaining a complete new data file from NASA/LRC, and attaching it to the program. The letter of transmittal is attached.

Task 3.2g, Update Kinetic Data

The reaction rate study has been completed and the results were sent to the COR at NASA/MSFC in September.

3.3 NOZZLE SHOCK WAVES

The plan for doing Task 3.3c, multiple shock waves, has been approved by the COR. A small amount of work was done on this task during the quarter.

3.4 VERIFICATION

No work was done on this task during the reporting period.

3.5 DOCUMENTATION

Work was begun on this task near the end of the reporting period.

4.0 WORK PLANNED FOR THE NEXT REPORTING PERIOD

All remaining work is to be completed during the next reporting period.

5.0 CURRENT PROBLEM AREAS

The rate of spending on the contract is too low, about 20% per quarter rather than 25% per quarter. It is clear that a time extension will be necessary. A revised schedule is being prepared.

6.0 COST STATUS

As of the end of the reporting period, the cost status of this contract is as follows:

1) Total Cumulative Costs through 30 September 1984	$63,300
2) Estimated Cost to Complete	$55,700
3) Estimated Percentage of Physical Completion of the Contract	55%

The costs on the contract to date correspond well with the estimated percentage of completion.

APPENDIX A

NUMERICAL INTEGRATION IN ODK

Given a differential equation of the form $\frac{dy}{dx} = f(x,y)$, a family of implicit integration schemes is based on the following back-differencing differentiation formula.[1]

$$\nabla y_{n+1} + \frac{1}{2}\nabla^2 y_{n+1} + \frac{1}{3}\nabla^3 y_{n+1} + \ldots = y'_{n+1}h,$$

where

$$\nabla y_{n+1} = y_{n+1} - y_n ,$$

$$\begin{aligned}\nabla^2 y_{n+1} &= \nabla y_{n+1} - \nabla y_n \\ &= y_{n+1} - y_n + y_n - y_{n-1} \\ &= y_{n+1} - 2y_n + y_{n-1},\end{aligned}$$

$$\nabla^3 y_{n+1} = \nabla(\nabla^2 y_{n+1}), \text{ etc.}$$

$$h = x_{n+1} - x_n$$

For example, using one term in the sum on the left gives $y_{n+1} = y_n + hy'_{n+1}$, which is the usual backward Euler method.

In general, using the first k terms gives an implicit method of order k, with a local error approximately equal to the (k+1) term.

Thus, using the first two terms gives

$$\nabla y_{n+1} + \frac{\nabla y_{n+1} - \nabla y_n}{2} = hy'_{n+1} ,$$

or

$$\frac{3}{2}\nabla y_{n+1} - \frac{1}{2}\nabla y_n = hy'_{n+1} , \qquad (1)$$

with a local error approximated by

$$\frac{1}{3}\nabla^3 y_{n+1} = \frac{1}{3}(\nabla y_{n+1} - 2\nabla y_n + \nabla y_{n+1}). \qquad (2)$$

Ref. 1 Dahlquist, G., and Bjorck, A., Numerical Methods, Prentice-Hall, 1974. (see equation 8.3.12).

The integration method used in ODK is a variation of the above second order method in that y'_{n+1} is approximated by

$$y'_{n+1} = f(x_{n+1}, y_{n+1}) \tag{3}$$

$$= f(x_n, y_n) + \frac{\partial f}{\partial x}(x_n, y_n)(x_{n+1} - x_n)$$

$$+ \frac{\partial f}{\partial y}(x_n, y_n)(y_{n+1} - y_n)$$

From (1) and (2),

$$\frac{3}{2} k_{n+1} - \frac{1}{2} k_n = h(f_n + \alpha_n h + \beta_n k_{n+1}) \tag{4}$$

with

$$\alpha_n = \frac{\partial f}{\partial x}(x_n, y_n) \quad ,$$

$$\beta_n = \frac{\partial f}{\partial y}(x_n, y_n) \quad ,$$

$$k_n = \nabla y_n = y_n - y_{n-1} \ ,$$

$$k_{n+1} = \nabla y_{n+1} = y_{n+1} - y_n, \text{ and}$$

$$f_n = f(x_n, y_n).$$

Solving for k_{n+1} ,

$$(1 - \frac{2}{3} \beta_n) k_{n+1} = \frac{1}{3}(k_n + 2(f_n + \alpha_n h)h) \tag{5}$$

The procedure can be extended easily for a system of n equations in n dependent variables.

Given

$$\frac{dy_i}{dx} = f(x, y_i, \ldots, y_n) \ , \ i=1, \ldots, n,$$

equation (1) becomes

$$\frac{3}{2} \nabla y_{i,n+1} - \frac{1}{2} \nabla y_{i,n} = hy'_{i,n+1} \quad , \ i=1, \ldots, n$$

equation (3) becomes

$$y'_{i,n+1} = f_i(x_{n+1}, y_{1,n+1}, \ldots, y_{n,n+1})$$

$$= f_i(x_n, y_{1,n}, \ldots, y_{n,n}) + \frac{\partial f_i}{\partial x}(x_n)(x_{n+1} - x_n)$$

$$+ \sum_{j=1}^{n} \frac{\partial f_i}{\partial y_j}(x_n)(y_{j,n+1} - y_{j,n})$$

equation (4) becomes

$$\frac{3}{2} k_{i,n+1} - \frac{1}{2} k_{i,n} = h \left(f_{i,n} + \alpha_{i,n} h + \sum_{j=1}^{n} \beta_{i,j,n} k_{j,n}\right) \qquad i=1,\ldots,n$$

and equation (5) becomes

$$\left(1 - \frac{2}{3} \beta_{i,i,n}\right) k_{i,n+1} = \frac{1}{3} \left(k_{i,n} + 2 \left(f_{i,n} + \alpha_{i,n} h + \sum_{\substack{j \neq i \\ j=1}}^{n} \beta_{i,j,n} k_{j,n}\right)\right)$$

The maximum local error is defined by equation (2),

$$\max_{1 \leq i \leq n} \frac{1}{3} \left(k_{i,n+1} - 2 k_{i,n} + k_{i,n-1}\right).$$

APPENDIX B

6.1.1 THERMODYNAMIC DATA BELOW 300°K.

If the temperature at any point computed by ODE, ODK, or TDK is found to be below the Thermodynamic Data lower temperature limit, T_ℓ, the polynomial curve fit data (see Section 6.1) will be extrapolated to obtain values for the thermodynamic data. The extrapolated data can be inaccurate. The LØW T CPHS data set can be used to input low temperature data for those species for which extrapolation of the JANNAF data is not accurate. Only Cp vs. T is input. Enthalpy and entropy are obtained by integrating Cp vs. T within the computer program.

The lower temperature limit, T_ℓ, in the Thermodynamic Data supplied with the program is 300°K. Thermodynamic Data below the temperature, T_ℓ, may be input by data cards as described in Table 6-5.

An example of this input is given in Table 6-6 which shows a card listing extending the Thermodynamic Data for an O_2/H_2 propellant to 100°K. Data in Table 6-6 is taken directly from the JANAF tables (Reference 23), except for Argon which is taken from NASA SP-3001.

Ref. 23 Stull, D.R., Prophet, H., et al., JANAF Thermochemical Tables, Second Edition, NSRDS-NBS 37, National Standard Reference Data Series, National Bureau of Standards, June 1971.

Table 6-5: Input Specifications for Low Temperature Thermodynamic Data.

The first card is a directive card that identifies the start of the low temperature thermodynamic data input. It reads as follows, columns 1 through 10:

```
LOW T CPHS
```

The next card contains a species name consisting of 12 characters, or less, left justified to column 1. An integer is placed in column 21 indicating the number of T, Cp values that follow. A value of 1,2, or 3 can be used. For example:

```
H2O                 2
```

Next, the thermodynamic data for the species named above is input. There must be one pair of T, Cp values per card. These cards are numbered consequently in column 45. They are read as 2F10.0,20X,I5. For example, for H_2O:

```
100.                    7.961                        1
200.                    7.969                        2
```

Species name cards and thermodynamic data cards for other species, if any, follow.

A final directive card is used to identify the end of the low temperature thermodynamic data. It reads as follows, columns 1 through 14:

```
END LOW T CPHS
```

TABLE 6-6. LOW TEMPERATURE $C^O_{p_T}, H^O_T, S^O_T$ DATA FOR AN O_2/H_2 PROPELLANT

col.no. |1 |21 |45

```
LOW T CPHS
AR                  2
100.0      4.9681                          1
200.0      4.9681                          2
H                   2
100.0      4.968                           1
200.0      4.968                           2
H2                  2
100.0      5.393                           1
200.0      6.518                           2
H2O                 2
100.0      7.961                           1
200.0      7.969                           2
N2                  2
100.0      7.074                           1
200.0      6.989                           2
O                   2
100.0      5.666                           1
200.0      5.434                           2
OH                  2
100.0      7.567                           1
200.0      7.309                           2
O2                  2
100.0      6.958                           1
200.0      6.961                           2
END LOW T CPHS
```